

**MASSACHUSETTS INSTITUTE OF TECHNOLOGY**  
 Department of Civil and Environmental Engineering

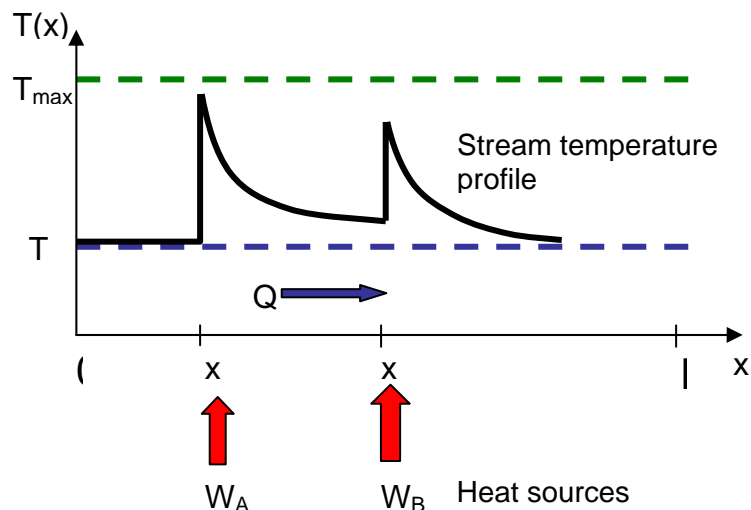
**1.731 Water Resource Systems**

**Lecture 11, Differential Constraints and Response Matrices, Oct. 5, 2006**

Standard formulation of optimization problem relies on **algebraic constraints**. In many environmental applications constraints arise most naturally as **differential equations**. How should these differential constraints be handled?

**Example – Allocation of waste heat discharges along a stream**

Problem is to select heat discharges  $W_A$  and  $W_B$  at 2 locations  $x_A$  and  $x_B$  along stream in order to maximize total heat discharged  $W_A + W_B$ , subject to upper limit ( $T_{max}$ ) on water temperature  $T$ .



Incorporate model based on **stream energy balance** (relates heat discharges and stream temperature):

$$\frac{dE}{dt} = 0 = \rho\gamma Q \frac{dT}{dx} + k_e A \rho \gamma (T - T_0) + W_A \delta(x - x_A) + W_B \delta(x - x_B) \quad ; \quad T(0) = T_0$$

$E$  = Energy per unit length [Joules/m]

$\rho$  = Density of water [ $\text{kg}/\text{m}^3$ ]

$\gamma$  = Specific heat of water [Joules/( $\text{kg} \cdot ^\circ\text{C}$ )]

$Q$  = Stream flow [ $\text{m}^3/\text{day}$ ]

$T$  = Water temperature [ $^\circ\text{C}$ ]

$T_0$  = Air temperature [ $^\circ\text{C}$ ]

$A$  = Stream cross-section [ $\text{m}^2$ ]

$k_e$  = Exchange rate [1/day]

$W_A, W_B$  Source heat flux [Joules/ day]

$\delta(x - x_A), \delta(x - x_B)$  = Dirac delta function at  $x_A$  or  $x_B$  [1/m], defined by:

$$\int_{x_L}^{x_U} f(x)\delta(x - x')dx = f(x') \quad x_L < x' \leq x_U$$

$$= 0 \quad \text{otherwise}$$

Assume steady state ( $dE/dt = 0$ ) and simplify to:

$$\frac{dT}{dx} = -\alpha(T - T_0) + W_A\delta(x - x_A) + W_B\delta(x - x_B) \quad ; \quad T(0) = T_0$$

$$\alpha = \frac{k_e A}{Q} \quad \beta = \frac{1}{\rho\gamma Q}$$

Suppose solution to this equation at any  $x$  is  $T(x, W_A, W_B)$ . Then optimization problem is:

$$\text{Maximize } W_A + W_B$$

$W_A, W_B$

such that :

$$T(x, W_A, W_B) \leq T_{max} \quad ; \quad \forall x$$

Note that the temperature constraint as given here is evaluated at **every  $x$**  (infinite number of algebraic constraints).

There are three ways to write the constraint  $T(x, W_A, W_B) \leq T_{max}$  in a practical (finite) form:

1. **Analytical solution** -  $T(x, W_A, W_B)$  is written as an **explicit** function of  $W_A$  and  $W_B$ .
2. **Imbedding** -  $T(x, W_A, W_B)$  is defined **implicitly**, by a set of discretized model equations.
3. **Response matrix** -  $T(x, W_A, W_B)$  is approximated by a Taylor series expressed in terms of model sensitivity derivatives.

### Analytical solution

Solution to stream equation with upstream boundary condition imposed:

$$T(x, W_A, W_B) = T_0 + \beta W_A \int_0^x e^{-\alpha(x-\xi)} \delta(\xi - x_A) d\xi + \beta W_B \int_0^x e^{-\alpha(x-\xi)} \delta(\xi - x_B) d\xi$$

Apply definition of  $\delta$  function to get:

$$T(x, W_A, W_B) = T_0 \quad x \leq x_A$$

$$T(x, W_A, W_B) = T_0 + \beta W_A e^{-\alpha(x-x_A)} \quad x_A < x \leq x_B$$

$$T(x, W_A, W_B) = T_0 + \beta W_A e^{-\alpha(x-x_A)} + \beta W_B e^{-\alpha(x-x_B)} \quad x > x_B$$

Note that temperature is highest at the discharge points  $x_A$  and  $x_B$ . Therefore, we can apply temperature constraint only at  $x_A$  and  $x_B$  rather than at all points  $x$ :

$$\text{Maximize } W_A + W_B \\ W_A, W_B$$

such that :

$$T_0 + \beta W_A - T_{max} \leq 0 \quad \text{at } x_A \\ T_0 + \beta W_A e^{-\alpha(x_B - x_A)} + \beta W_B - T_{max} \leq 0 \quad \text{at } x_B$$

This is in standard form, with algebraic rather than differential constraints. This approach is best when analytical solution is available, but that is not usually the case.

### Imbedding

When an analytical solution is not available an approximate numerical solution can be obtained by discretizing the differential equation over a computational grid of equally spaced points  $x_1, x_2, \dots, x_N$ .

In this example use either of two approximations for the spatial derivative at each computational grid point:

$$\left. \frac{\partial T}{\partial x} \right|_{x_i} \approx \frac{T(x_{i+1}) - T(x_i)}{\Delta x} = \frac{T_{i+1} - T_i}{\Delta x} \quad \text{Forward difference (explicit)} \\ \left. \frac{\partial T}{\partial x} \right|_{x_i} \approx \frac{T(x_i) - T(x_{i-1})}{\Delta x} = \frac{T_i - T_{i-1}}{\Delta x} \quad \text{Backward difference (implicit)}$$

The Dirac delta function is approximated by  $1/\Delta x$ .

The **explicit discretization** yields a set of  $N$  coupled equations as follows:

$$T_i = T_0 \quad x_i = x_0 \\ T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) \quad x_0 < x_i \leq x_A \\ T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) + \beta W_A \quad x_A < x_i \leq x_B \\ T_{i+1} = T_i - \alpha \Delta x (T_i - T_0) + \beta W_B \quad x_i > x_B$$

These **first-order difference equations** have the same general form as the reservoir storage equation in Problem Set 3.

The system of equations obtained from the **implicit discretization** is most conveniently expressed in matrix form:

$$A_{ki} T_i = b_k(W_A, W_B) \quad i, k = 1, \dots, N$$

$$\text{where } A_{ii} = 1 \quad \text{for } i = 1, \dots, N \\ A_{i,i-1} = \alpha \Delta x - 1 \quad \text{for } i = 2, \dots, N \\ A_{i,k} = 0 \quad \text{otherwise}$$

$$\begin{aligned}
b_i &= T_0 && \text{for } i=1 \\
b_i &= \alpha \Delta x T_0 && \text{for } i > 1 \text{ and } x_i \neq x_A \text{ or } x_B \\
b_i &= \beta W_A + \alpha \Delta x T_0 && \text{for } x_i = x_A \\
b_i &= \beta W_B + \alpha \Delta x T_0 && \text{for } x_i = x_B
\end{aligned}$$

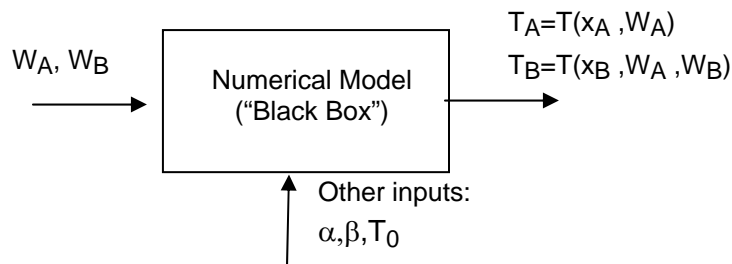
Both the explicit and implicit discretizations are in a form that can be inserted directly into optimization software such as GAMS (note that the implicit matrix equation does need not be solved and the decision variables only appear on the right-hand side – the implicit constraints relating each  $T_i$  to  $W_A$  and  $W_B$  are sufficient).

The disadvantage of imbedding is the **large number of decision variables and constraints** it produces (one for each grid point for each scalar differential equation). This is particularly inefficient in the example problem since we really only care about the temperature solutions at the two points  $x_A$  and  $x_B$ . Solutions at all the other upstream points need to be computed in order to obtain these two temperatures.

### Response Matrix

Response matrix methods represent differential constraints with efficient linear approximations.

Assume we have a numerical model available to evaluate temperatures  $T(x_A, W_A)$  and  $T(x_B, W_A, W_B)$  at the discrete locations  $x_A$  and  $x_B$ , for any set of decision variables  $W_A$  and  $W_B$ .



Expand these temperatures in a Taylor series around nominal decision values (e.g.  $W_A = W_B = 0$ ):

$$\begin{aligned}
T(x_A, W_A) &= T(x_A, 0) + \boxed{\frac{\partial T(x_A, W_A)}{\partial W_A} \Big|_{W_A=0}}^{R_{AA}} W_A + \dots \\
T(x_B, W_A, W_B) &= T(x_B, 0, 0) + \boxed{\frac{\partial T(x_B, W_A, 0)}{\partial W_A} \Big|_{W_A=0}}^{R_{BA}} W_A + \boxed{\frac{\partial T(x_B, 0, W_B)}{\partial W_B} \Big|_{W_B=0}}^{R_{BB}} W_B + \dots
\end{aligned}$$

Associate the sensitivity derivatives with the elements of a response matrix  $R$  and rearrange equations:

$$\begin{bmatrix} T_0 \\ T_0 \end{bmatrix} + \begin{bmatrix} R_{AA} & 0 \\ R_{BA} & R_{BB} \end{bmatrix} \begin{bmatrix} W_A \\ W_B \end{bmatrix} = \begin{bmatrix} T_A \\ T_B \end{bmatrix}$$

Resulting constraints for the optimization problem are:

$$\begin{bmatrix} T_0 \\ T_0 \end{bmatrix} + \begin{bmatrix} R_{AA} & 0 \\ R_{BA} & R_{BB} \end{bmatrix} \begin{bmatrix} W_A \\ W_B \end{bmatrix} \leq \begin{bmatrix} T_{\max} \\ T_{\max} \end{bmatrix}$$

In this example the response matrix approximation is **exact** because the differential constraints are **linear** in the decision variables. Consequently, the response matrix elements can be identified directly from the analytical solutions above.

More generally, we derive the sensitivity derivatives numerically, from multiple model evaluations. For example:

$$R_{BA} \approx \frac{T(x_B, \varepsilon, 0) - T(x_B, 0, 0)}{\varepsilon}$$

This approach does not require knowledge of the model equations (i.e. the model can be a “black box”).

The response matrix approach can also be used to approximate **nonlinear** differential constraints, so long as the Taylor series expansion is sufficiently accurate.